Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supplemental Materials

GC-MS metabolomics on PPARα-dependent exacerbation of colitis

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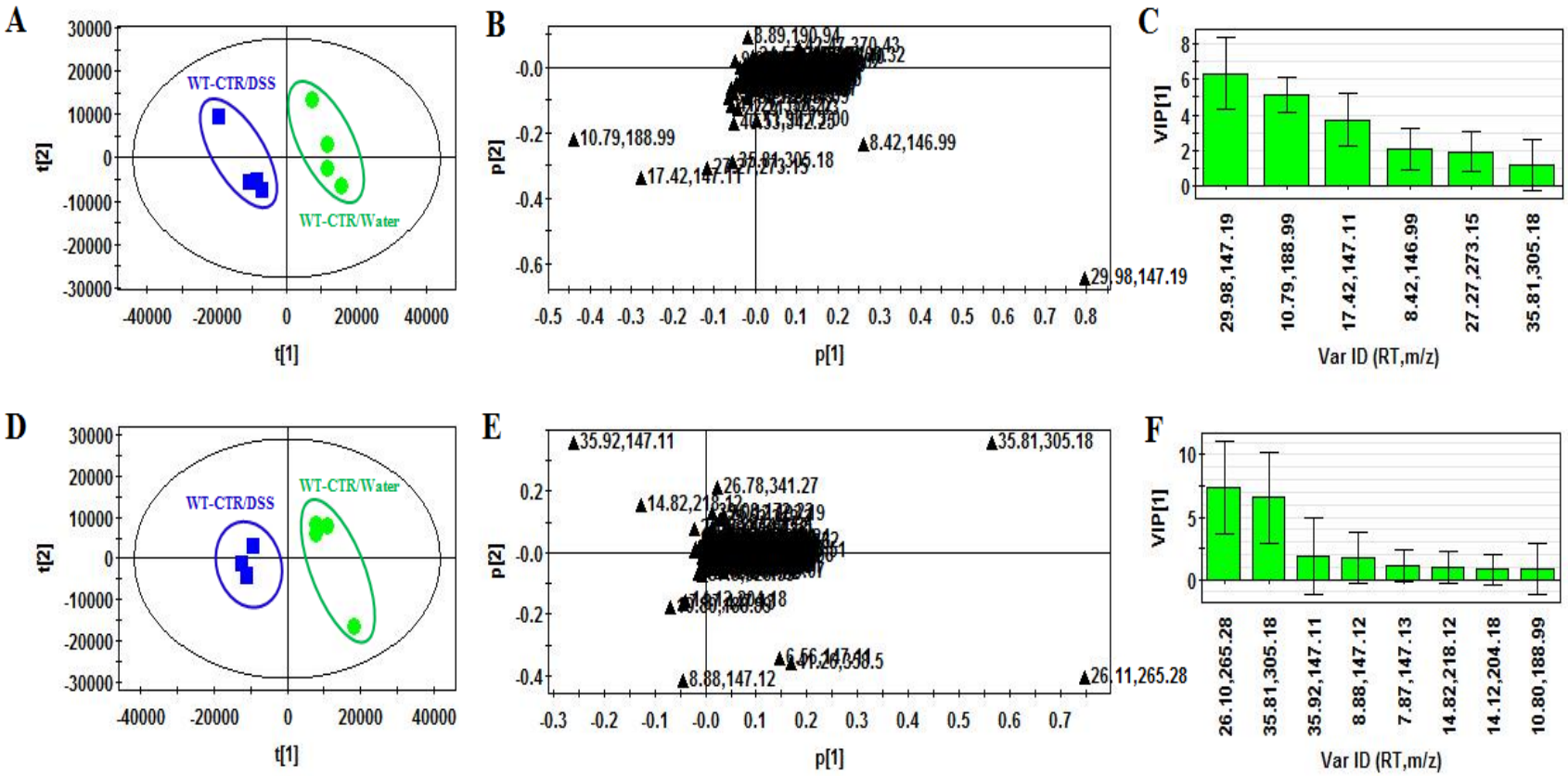

Figure S1. PLS-DA models discriminating the control and colitis groups for serum (A-C) and colon (D-F). (A) PLS-DA score plot of the first two latent variables (serum, with the cumulative R^2X 0.617, R^2Y 0.968, and Q^2 0.935); (B) PLS-DA loading plot explaining separation in (A) and the associated VIP plot of the first component highlighting discriminatory metabolite markers (C); (D) PLS-DA score plot of the first two latent variables (colon, with the cumulative R^2X 0.732, R^2Y 0.995, and Q^2 0.958); (E) PLS-DA loading plot explaining separation in (D) and the associated VIP plot of the first component highlighting discriminatory metabolite markers (F).

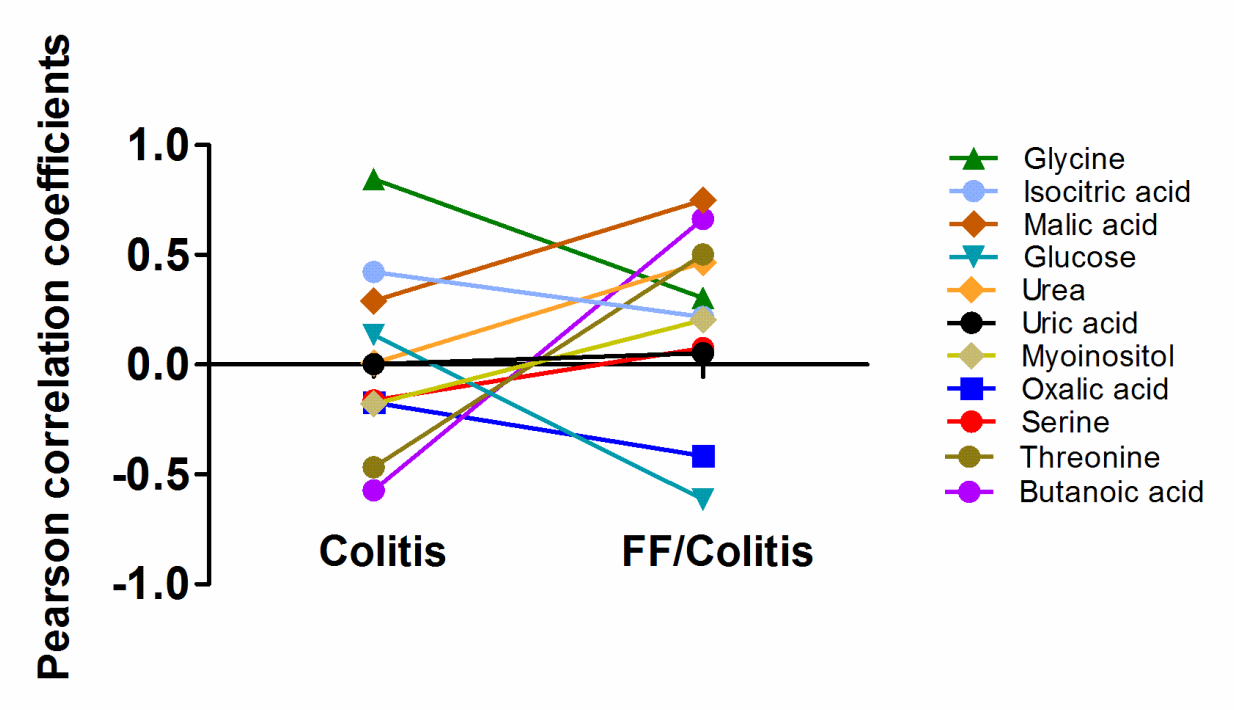

Figure S2. Pearson correlation coefficients of the levels of the metabolite markers in serum and colon, for the colitis mice and fenofibrate/DSS-treated WT mice (FF/colitis).

Table.S1 Body weight changes of the mice in the four examined groups*

(% Initial body weight, mean±SD, n=4 for each group)

Days	WT-CTR/Water	WT-CTR/DSS	WT-FF/DSS	KO-FF/DSS
0	100.00±0.00	100.00±0.00	100.00±0.00	100.00±0.00
1	101.77±0.21	99.12±1.19$^{\#\#}$	97.65±0.64	99.19±0.70
2	103.90±0.20	100.60±1.20$^{\#\#}$	96.20±0.90^{++}	100.90±0.80$^{\Delta\Delta}$
3	104.00±0.00	98.00±1.00$^{\#\#}$	95.00±1.00^{++}	99.00±1.00$^{\Delta\Delta}$
4	103.85±0.47	101.88±1.00$^{\#\#}$	95.15±1.40^{++}	99.77±1.31$^{\Delta\Delta}$
5	103.89±0.77	98.55±1.49$^{\#\#}$	93.90±1.00^{++}	95.64±2.26
6	103.99±0.58	95.93±1.73$^{\#\#}$	84.09±2.76^{++}	92.26±2.51$^{\Delta}$
7	104.63±0.63	87.17±2.21$^{\#\#}$	77.26±1.73^{++}	85.81±1.85$^{\Delta\Delta}$

$^{\#\#}$ p <0.01, comparing WT-CTR/Water and WT-CTR/DSS groups; $^{++}$ p < 0.01, comparing WT-CTR/DSS and WT-FF/DSS groups; $^{\Delta\Delta}$ p < 0.01 and $^{\Delta}$ p < 0.05, comparing WT-FF/DSS and KO-FF/DSS groups.

*Figures of these body weight changes could be found in our publication (American Journal of Physiology - Gastrointestinal and Liver Physiology, 2014, 307, G564-G573).

Table.S2 Metabolic pathway enrichment analysis of the metabolites identified as potential biomarkers

Pathway name	*P* value	Adj. *P* value	Hits	Metabolites
Purine metabolism	0.002800	0.017733	3	Uric acid, Glycine, Urea
Glyoxylate and dicarboxylate metabolism	0.000322	0.005623	3	Malic acid, Isocitric acid, Oxalic acid
Aminoacyl-tRNA biosynthesis	0.001553	0.013644	3	Threonine, Serine, Glycine
Glycine, serine and threonine metabolism	0.000444	0.005623	3	Glycine, Threonine, Serine
Galactose metabolism	0.007462	0.028356	2	Glucose, Myoinositol
Citrate cycle (TCA cycle)	0.001795	0.013644	2	Isocitric acid, Malic acid

P-value, statistically assessed against the background set; adj. *p*-value, *p*-value corrected using the false discovery rate.